

Electronic Supplementary Information

Computational-Aided Design of Melatonin Analogues with Outstanding Multifunctional Antioxidant Capacity

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Table S1. Gibbs energies of reaction (ΔG , kcal/mol), Gibbs energies of activation (ΔG^\ddagger , kcal/mol), imaginary frequencies (if , cm^{-1}), tunneling corrections (κ), and rate constants for each individual HT reaction path (k_i^{HT} , $\text{M}^{-1}\text{s}^{-1}$), at 298.15 K, for the HT reactions of melatonin analogues in test set 1 with $\cdot\text{OOH}$.

	ΔG	ΔG^\ddagger	if	κ	k_i^{HT}
Ia	-7.08	12.61	3027.8	277.07	9.81E+05
Ib	-7.42	12.25	2965.3	219.02	1.43E+06
Ic	-7.77	12.41	3731.3	316.72	1.58E+06
IIa-site3	-10.21	11.57	2025.4	17.35	3.58E+05
IIa-site4	-10.88	10.88	2049.3	17.11	1.11E+06
IIb-site3	-12.18	9.29	1828.5	4.04	3.90E+06
IIb-site6	-14.54	9.59	2147.0	4.80	2.79E+06
IIc-site4	-11.11	10.28	2251.3	11.76	2.13E+06
IIc-site5	-13.61	9.84	2175.6	7.88	2.99E+06
IIIa-site3	-9.53	11.58	2149.5	24.65	4.98E+05
IIIa-site4	-13.10	10.24	1837.6	4.33	8.39E+05
IIIa-site5	-11.94	12.01	2275.7	15.35	1.49E+05
IIIb-site3	-14.39	7.67	1516.3	1.48	2.19E+07
IIIb-site4	-10.02	11.52	2578.1	44.76	9.93E+05
IIIb-site6	-13.45	10.15	2306.8	8.96	2.01E+06

Table S2. Reorganization energy (λ , kcal/mol) and Gibbs energies of activation (ΔG^\ddagger , kcal/mol), at 298.15 K, for the SPLET reactions of melatonin analogues in test set 1 with $\cdot\text{OOH}$.

	λ	ΔG^\ddagger
Ia	15.48	2.00
Ib	15.18	2.56
Ic	14.64	1.85
IIa	16.68	2.12
IIb	15.83	0.86
IIc	16.18	1.35
IIIa	14.48	2.17
IIIb	17.54	1.43

Table S3. Gibbs energies of reaction (ΔG , kcal/mol), Gibbs energies of activation (ΔG^\ddagger , kcal/mol), imaginary frequencies ($i f$, cm^{-1}), tunneling corrections (κ), and rate constants for each individual HT reaction path (k_i^{HT} , $\text{M}^{-1}\text{s}^{-1}$), at 298.15 K, for the HT reactions of melatonin analogues in test set 3 with $\cdot\text{OOH}$.

	ΔG	ΔG^\ddagger	$i f$	κ	k_i^{HT}
IbD	-6.26	13.92	2615.4	212.46	2.47E+05
IbG	-6.08	13.56	2546.7	175.52	4.97E+05
IIcD-site4	-9.79	10.35	2216.2	25.69	2.06E+07
IIcD-site5	-12.53	9.15	1820.8	7.51	5.42E+07
IIcG-site4	-9.74	11.76	2224.6	27.78	3.27E+06
IIcG-site5	-12.63	10.77	1869.5	9.00	6.34E+06

Table S4. Reorganization energy (λ , kcal/mol) and Gibbs energies of activation (ΔG^\ddagger , kcal/mol), at 298.15 K, for the SPLET reactions of melatonin analogues in test set 3 with $\cdot\text{OOH}$.

	λ	ΔG^\ddagger
IbD	15.63	3.59
IbG	14.73	3.87
IIcD	16.23	2.26
IIcG	16.21	2.29

Table S5. Conditional Gibbs free energies of reaction ($\Delta G'$, kcal/mol) and conditional equilibrium constants (K' , M), at pH=7.4, for all the γ Cu(II) chelation routes by melatonin analogues in test set 3.

	$\Delta G'$	K'
IbD -c1	-5.38	8.8E+03
IbD -c2	3.42	3.1E-03
IbG -c1	-7.52	3.2E+05
IbG -c2	1.44	8.7E-02
IIcD -c1	-6.39	4.9E+04
IIcD -c2	4.54	4.7E-04
IIcD -c3	-5.48	1.0E+04
IIcG -c1	-6.47	5.5E+04
IIcG -c2	-0.81	3.9E+00
IIcG -c3	-3.83	6.4E+02

Optimized geometries of the transition states

TS-la

```
\\O,-3.181200904,-1.6235450551,-0.4207058317\N,2.1385841573,2.1459
069217,0.1546688214\N,-3.5038332487,0.3891605036,0.548392157\C,0.09351
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44134,0.082777175\C,0.8185069877,2.4433961448,-0.0414982525\C,-2.08858
68366,0.6372064112,0.7787039011\C,0.9081189722,-1.1837447701,-0.292596
688\C,3.4494261435,0.0135918082,0.2039843128\C,2.0313663767,-1.9624845
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70822,1.1070777232,0.7808019926\H,-5.971172558,0.0417422506,0.09984536
38\H,-5.7881894659,-1.7247105468,0.2059534938\H,-5.6085938462,-0.91967
57104,-1.3526424984\H,1.9830526867,-3.0390275208,-0.2531039821\O,4.387
4817833,-2.1698645316,0.1404122387\H,4.6925728088,-2.2500071412,1.1445
124124\O,4.7215568292,-2.2171779935,2.5369760977\O,3.5893806364,-1.536
3270979,2.8059378456\H,3.8376316329,-0.5966426522,2.8253585633\\
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TS-lb

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TS-lc

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TS-IIa (site 3)

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3946543714,-0.3890945899\\O,2.1045160761,-2.8803535773,-0.1180364607\\H,
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4080621896,0.7582402179\H,5.812757358,-0.3633456529,0.2251638311\H,5.6
929497354,1.3839996295,0.5344136236\H,5.5411864418,0.7766906944,-1.113
4270908\H,-4.6067224548,-1.0071730754,0.4430519781\O,-2.4717472841,2.9
689640775,0.111253201\H,-1.5868775599,3.2865654949,-0.1185080525\H,-4.
5592492329,1.4858272783,0.4880920656\O,-0.1451919055,1.659091604,-0.41
27640068\H,0.2500354775,1.9939755842,0.4776905387\O,0.34201576,2.33035
68945,1.9124997938\O,-0.6424021612,1.5608373107,2.3954522631\H,-1.4037
899361,2.1502310572,2.5388577807\\

TS-IIc (site 4)

\\O,-3.502289136,-1.571103533,-0.4351040794\N,1.8983000574,2.05907503
31,0.0793157617\N,-3.7828568963,0.4264961821,0.5784665432\C,-0.1805582
688,1.2672217029,-0.2636781719\C,0.7228889588,0.1582069986,-0.19864664
46\C,-1.6616892026,1.1929294424,-0.4574404333\C,2.0096184297,0.6951207
91,0.0138362359\C,0.5815690848,2.3973824216,-0.0863424387\C,-2.3611649
925,0.6509706794,0.7937023432\C,0.5513475268,-1.2401020649,-0.31467313
1\C,3.1308126518,-0.1218987352,0.1184600829\C,1.6527084514,-2.05283831
72,-0.2018602625\C,2.9382489262,-1.5080861433,0.0169265153\C,-4.250934
2423,-0.65969804,-0.0460854215\C,-5.7354345166,-0.7369434112,-0.253143
0462\H,-2.0553413898,2.1827479384,-0.689122869\H,-1.8933509983,0.53479
49113,-1.297035236\H,0.2774030312,3.4308100826,-0.0716691399\H,-2.2579
154353,1.3563407368,1.6148484674\H,-1.9080758087,-0.2908659078,1.09767
59684\H,2.6589237756,2.7054128189,0.216703007\H,-4.4368740378,1.148141
4378,0.8343994373\H,-6.2634766306,0.1101066007,0.1778228003\H,-6.09831
41456,-1.6617946981,0.193459378\H,-5.930147323,-0.7813806626,-1.324419
4716\H,1.5717307991,-3.1283561565,-0.2803349164\H,-0.4314422381,-1.658
2712858,-0.4867800454\O,4.0365060477,-2.299807185,0.0930871215\H,4.281
7207467,-2.4366643557,1.0883752591\O,4.3560272391,0.4144797778,0.32646
03702\H,5.0124242703,-0.2975894291,0.3090888168\O,4.2950710219,-2.3147
023578,2.537493404\O,3.217490513,-1.5381849703,2.7263271381\H,3.547633
3807,-0.625247602,2.7945191469\\

TS-IIc (site 5)

\\O,-3.4023976229,-1.6079699859,-0.2474192197\N,1.9225959771,2.143772
9307,-0.0073936366\N,-3.7154736298,0.4494212099,0.6264279122\C,-0.1431
424626,1.3053470576,-0.3145125226\C,0.7927030305,0.2161211381,-0.22430
95918\C,-1.6235153541,1.187668331,-0.4877505885\C,2.0657453132,0.78895
11575,-0.039527945\C,0.5900423004,2.4532569113,-0.1754463698\C,-2.2955
348633,0.7131304383,0.8054866498\C,0.6721256672,-1.1823700492,-0.29711
38606\C,3.2209018401,0.0056757658,0.0798166244\C,1.8015518114,-1.97175
4343,-0.183412837\C,3.060938698,-1.3863784906,0.0059902004\C,-4.165915
671,-0.6833256065,0.0750496452\C,-5.6483277122,-0.7954900415,-0.129548
7808\H,-2.039572444,2.15238088,-0.7782723413\H,-1.8499777198,0.4719323
734,-1.2803299363\H,0.2662132774,3.4805528315,-0.1879212111\H,-2.19198
0964,1.4709846815,1.5784587975\H,-1.8200082586,-0.1997201987,1.1594494
581\H,2.6722442207,2.8085147354,0.0988715214\H,-4.3777890314,1.1841007
204,0.8175793441\H,-6.1860434195,0.0779782434,0.2306976083\H,-6.002320
0265,-1.685137939,0.3900353829\H,-5.8384962931,-0.9281611451,-1.194242
6255\H,1.7391166756,-3.0497063707,-0.2347687425\H,-0.2978660606,-1.640
4627665,-0.4404763109\O,4.1514470077,-2.1896696959,0.1176571868\H,4.93
63922771,-1.6319855835,0.2186696238\O,4.4533608058,0.5381664762,0.2293
881428\H,4.6183258451,0.6957932158,1.236061946\O,4.4311070244,0.601660
0068,2.6873374953\O,3.4536946453,-0.3126736101,2.7455209783\H,2.616060
2064,0.1808581714,2.7920847928\\

TS-IIIa (site 3)

\\O,3.4503257435,1.5548437231,-0.3291390696\N,-1.6813186473,-2.44753
69662,-0.0853952806\N,3.8646399175,-0.4750870113,0.565241285\C,0.34998
3465,-1.5237314194,-0.3912686041\C,-0.628621528,-0.4699946958,-0.25016
2461\C,1.8221630797,-1.328922181,-0.5631841279\C,-1.880215409,-1.10361
68335,-0.0594290898\C,-0.3339773371,-2.6985740485,-0.2835792741\C,2.46
00375943,-0.815653313,0.7327748062\C,-0.5514104704,0.9193827477,-0.273
4874256\C,-3.0659991122,-0.3793941417,0.1214169902\C,-1.7298676997,1.6
461698285,-0.0919252501\C,-2.9761448436,0.9917867127,0.1093782914\C,4.
2603470422,0.6817018665,0.0223245896\C,5.7390177043,0.8897534097,-0.12
97610693\H,2.2918466628,-2.270349107,-0.84814018\H,2.0123261894,-0.604
2312223,-1.357109443\H,0.0264419917,-3.7122853164,-0.3342182482\H,2.39
38806638,-1.5779197151,1.5054754607\H,1.9338499606,0.070141915,1.08448
95941\H,-2.3976506653,-3.1475911747,0.0237008903\H,4.5662636374,-1.159
6409831,0.795881799\H,6.3174842527,0.0318620967,0.2037808712\H,6.02244
95249,1.7684780889,0.4488216147\H,5.9537745842,1.0924093879,-1.1782863
152\H,0.3813162497,1.4484148694,-0.4174100854\O,-4.1166619068,1.724594
7338,0.2967175445\H,-3.8893541364,2.6603233301,0.2005303975\O,-4.24047
14117,-1.0530056474,0.3054907403\H,-4.9650937371,-0.4199170835,0.38662
40899\O,-1.7495936376,2.9940326535,-0.1260132046\H,-1.5009301712,3.360
2741435,0.8314412393\O,-1.2009791992,3.4313579606,2.1879708491\O,-0.90
44228287,2.1454598464,2.4489038207\H,-1.7323863024,1.7317521859,2.748296315\\

TS-IIIa (site 4)

\\O,3.4866919021,1.5836145978,-0.2635492193\\N,-1.6757989825,-2.39374
76282,0.0511611191\\N,3.9094820027,-0.4788937495,0.5503338242\\C,0.34254
3022,-1.4581338546,-0.2946307693\\C,-0.6259993363,-0.4105720507,-0.1935
211039\\C,1.8128977194,-1.2839782404,-0.5039882992\\C,-1.8745295274,-1.0
340452062,0.0161031097\\C,-0.3448012746,-2.6396027651,-0.1378811311\\C,2
.5088071786,-0.8050391254,0.774559598\\C,-0.522643346,0.996835746,-0.27
75583759\\C,-3.0390820076,-0.2894172701,0.141831495\\C,-1.6720166367,1.7
293421231,-0.1428524312\\C,-2.9317383967,1.1038115621,0.0679266315\\C,4.
2961591677,0.6832864733,0.0124552336\\C,5.7649880107,0.8586260813,-0.24
26348863\\H,2.2549547464,-2.2281489101,-0.8226925485\\H,1.9898482198,-0.
5488010329,-1.2917521819\\H,0.026679065,-3.6512029812,-0.1541738879\\H,2
.4653368949,-1.5802528634,1.5361006231\\H,2.0092856844,0.0804211543,1.1
639225755\\H,-2.3914794093,-3.0914734871,0.1736715621\\H,4.6079702008,-1
.1866199956,0.7100703782\\H,6.3547745726,0.0182332664,0.1150524993\\H,6.
0944466109,1.7745599053,0.2458383044\\H,5.9133734017,0.9759081446,-1.31
60838353\\H,0.4276551403,1.4872329164,-0.4387042291\\O,-4.049904088,1.86
04642045,0.1396894429\\H,-4.28212584,2.033488954,1.135496697\\O,-4.23267
38201,-0.8938424673,0.3463922958\\H,-4.9263396893,-0.2187302859,0.36519
01459\\O,-1.640256803,3.0981317943,-0.2045602294\\H,-2.5481235261,3.4251
677741,-0.1432591495\\O,-4.2309865461,1.9850095091,2.58056153\\O,-3.1025
854531,1.2877787942,2.7607831021\\H,-3.369164477,0.357325973,2.8671358705\\

TS-IIIa (site 5)

\\O,3.4183283492,1.5703514895,-0.310551786\\N,-1.7239777315,-2.4395335
759,-0.0426516673\\N,3.8212985684,-0.4435001646,0.6263165592\\C,0.298955
7804,-1.4920437068,-0.3154936313\\C,-0.6886468257,-0.4527330654,-0.2115
224182\\C,1.7726290913,-1.3005945554,-0.480940886\\C,-1.9313463643,-1.08
95838367,-0.0483446378\\C,-0.3796703573,-2.6786997503,-0.2056768482\\C,2
.4142466106,-0.7690354522,0.8057150401\\C,-0.6200440991,0.9522698936,-0
.2536336848\\C,-3.118355808,-0.3576789061,0.0893998444\\C,-1.7828616845,
1.6805402447,-0.1204124065\\C,-3.0205348637,1.0393141832,0.0540590638\\C
,4.2217396031,0.6917539591,0.0423182432\\C,5.6984958069,0.8668183103,-0
.1591039327\\H,2.2388943736,-2.2478819084,-0.7521677175\\H,1.9670503172,
-0.5887586551,-1.2854846727\\H,-0.0041786711,-3.6877614053,-0.235772413
7\\H,2.3426145661,-1.5147045444,1.5939933489\\H,1.8957594382,0.127616589
9,1.1401222297\\H,-2.4404421413,-3.1421426392,0.0476189634\\H,4.51627697
29,-1.1401836715,0.8421825705\\H,6.2734148683,0.024755186,0.2181249958\\
H,6.0095502665,1.7798377123,0.3473390205\\H,5.8875265855,0.9909796857,-
1.2249235199\\H,0.3217060227,1.469790801,-0.3826532097\\O,-4.1222257662,
1.8209429517,0.1859290596\\H,-4.9023232696,1.2532693176,0.2669487788\\O,
-4.3281009454,-0.934185464,0.2225059288\\H,-4.4595315071,-1.1783973483,
1.2239155069\\O,-1.7324858001,3.056298526,-0.1506895798\\H,-2.6249348314
,3.4097681823,-0.0534656412\\O,-4.2403523314,-1.1877240506,2.6521998322
\\O,-3.3083910313,-0.2284975286,2.7587362398\\H,-2.4463848121,-0.6803917
741,2.7567909077\\

TS-IIIb (site 3)

\\O,-3.370894242,-1.6213402005,-0.2014085841\N,1.7419728687,2.679567
0906,-0.0269278602\N,-3.6982531138,0.4720534259,0.578969661\C,-0.17927
79988,1.5549584505,-0.3589877633\C,0.9067352432,0.6164314263,-0.195851
2589\C,-1.633910989,1.2594379961,-0.55528329\C,2.0903238079,1.36426192
33,0.0059776181\C,0.3827974933,2.7935138595,-0.24631752\C,-2.283496688
9,0.7730598177,0.7442576905\C,1.0093027533,-0.7757604932,-0.2155529801
\C,3.3604999599,0.7924972496,0.1977994766\C,2.2622932075,-1.370406118,
-0.0218203018\C,3.4215217392,-0.5772773822,0.184222354\C,-4.1405361058
, -0.6918661963,0.0892176155\C,-5.6253046506,-0.834039446,-0.0818604188
\H,-2.1389256429,2.1680130021,-0.8849718694\H,-1.7715130551,0.50029984
62,-1.325996515\H,-0.080659389,3.7637662387,-0.3089644035\H,-2.1980714
223,1.5421627114,1.5088148994\H,-1.7802145127,-0.1222940829,1.10350207
46\H,2.3810834524,3.4515893417,0.0750487513\H,-4.3710267631,1.20145221
15,0.7505967772\H,-6.1675975584,0.0606593321,0.2138361744\H,-5.9608685
019,-1.6803161128,0.5165898439\H,-5.8313468513,-1.0575559419,-1.128082
8737\O,4.6146066527,-1.218431342,0.3711623724\H,4.4628081789,-2.170123
4758,0.2876683002\O,2.3827494178,-2.7195960811,-0.0731157874\H,2.12040
40242,-3.1143380092,0.8444378887\H,4.2465718401,1.3921372391,0.3480002
571\O,-0.0814795558,-1.5436430248,-0.4094804444\H,0.1840088376,-2.4745
195498,-0.4156344602\O,1.6807694344,-3.1760391458,2.2370768655\O,1.396
0349349,-1.8872097809,2.4547739083\H,2.2119943055,-1.4778478791,2.7933204323\\

TS-IIIb (site 4)

\\O,-3.4373637203,-1.6021398515,-0.2903395658\N,1.7325297172,2.6251455
739,0.0906247462\N,-3.7120760702,0.4674044944,0.5685277753\C,-0.161364
6753,1.4781518969,-0.3304311706\C,0.9153065168,0.5498533584,-0.1846876
337\C,-1.6155455637,1.1984873071,-0.5558477108\C,2.0934923127,1.298228
3573,0.0768937481\C,0.393430857,2.7260247346,-0.150954414\C,-2.2894396
191,0.7281199221,0.7371768063\C,1.0095059281,-0.8530684158,-0.26719124
57\C,3.3367090498,0.7154511067,0.2626935496\C,2.2334875929,-1.44871459
78,-0.0789527935\C,3.3944943524,-0.6777365278,0.1855594849\C,-4.184391
0664,-0.6689282694,0.0442989103\C,-5.6741192414,-0.7747491631,-0.10912
79878\H,-2.1018339295,2.112856432,-0.8971113581\H,-1.7504608018,0.4391
737995,-1.3257588698\H,-0.0874339366,3.6898298329,-0.1837910981\H,-2.1
852890886,1.4943563927,1.5022410721\H,-1.8112076792,-0.1802475527,1.09
93830021\H,2.3593673486,3.3976788583,0.2464242116\H,-4.3679253303,1.20
22724548,0.7787740263\H,-6.1943523505,0.1150298429,0.2375940369\H,-6.0
160225805,-1.6420925302,0.454634326\H,-5.9021816553,-0.9456414611,-1.1
606537697\O,4.5602046194,-1.3454431134,0.3105989819\H,4.7282663041,-1.
5458086591,1.3258301631\O,2.312260938,-2.8172090929,-0.1451922798\H,3.
2428634346,-3.0686669323,-0.0669186617\H,4.2332216023,1.287288248,0.45
56909937\O,-0.110032386,-1.587841005,-0.5297089694\H,0.1247159941,-2.5
239773112,-0.5696949008\O,4.5650964543,-1.6086381037,2.7254501365\O,3.
4080614741,-0.9407689097,2.8693977611\H,3.6464992783,-0.0047732456,2.9
863858472\\

TS-IIIb (site 6)

\\O,-3.2858738796,-1.6036776448,-0.1916544155\N,1.7557128814,2.723119
0076,-0.0625785721\N,-3.6560402037,0.4833088544,0.5857509419\C,-0.1636
923804,1.5979110771,-0.4029904843\C,0.9068646704,0.6596334265,-0.22215
84536\C,-1.6199254387,1.304649008,-0.5861787671\C,2.0894278624,1.39613
05995,-0.0102874345\C,0.4089727571,2.8413397612,-0.2954244219\C,-2.245
7719072,0.8170468953,0.7252659891\C,0.9934031869,-0.7458879281,-0.2267
523824\C,3.3371643331,0.8011940449,0.210083654\C,2.2412941752,-1.34527
43469,-0.0106130715\C,3.3950384018,-0.5764946984,0.2119463735\C,-4.075
8663054,-0.698307855,0.120158293\C,-5.5594635771,-0.8921504704,0.00136
98679\H,-2.1312080146,2.2109387752,-0.9118201219\H,-1.7648413187,0.541
3884594,-1.3517002933\H,-0.0516963958,3.8126534685,-0.3682986727\H,-2.
1652683316,1.5936446152,1.4828859595\H,-1.7193815248,-0.0648123991,1.0
843911013\H,2.3984680461,3.4914653865,0.0430012436\H,-4.3459331219,1.1
87303545,0.7925620645\H,-6.1222876986,-0.0198678796,0.3247776237\H,-5.
8417221766,-1.7543246188,0.6046278255\H,-5.796071101,-1.1153206097,-1.
0384592484\O,4.5973108035,-1.2038310231,0.4292363577\H,4.4697902486,-2
.1594709488,0.3846159347\O,2.3758771553,-2.7002411066,0.0068234156\H,1
.5317685884,-3.1023781259,-0.2443867147\H,4.2320109162,1.3847325805,0.
3759266815\O,-0.0585351879,-1.5461930561,-0.4833443934\H,-0.4220846976
, -1.9296848015,0.4104029013\O,-0.5002983754,-2.2861322331,1.8125343554
\O,0.4279194092,-1.461341307,2.3204097652\H,1.2334653706,-1.9954835118,
2.4363776884\

TS-IbF

\\O,-3.6919772739,-1.4677564895,0.3060422809\N,1.7984199118,1.700785
6475,-0.7643899702\N,-3.8499743021,0.756057053,0.6544800639\C,-0.38050
56571,1.1035455068,-0.8104843657\C,0.4346242196,-0.072727384,-0.716792
3537\C,-1.8749699457,1.0596280931,-0.8149638087\C,1.7780856641,0.35254
90359,-0.6923861962\C,0.4977532903,2.172791757,-0.8283234083\C,-2.4131
245268,0.9744581907,0.6205546515\C,0.1366311778,-1.4413610897,-0.65046
26245\C,2.8465045617,-0.5649015992,-0.5811327966\C,1.1844880055,-2.348
948242,-0.5495950942\C,2.5138956969,-1.9217569031,-0.5061282769\C,-4.3
901379103,-0.4542484096,0.4655941925\C,-5.8883329198,-0.5349430461,0.4
625531986\H,-2.3049355684,1.9206561408,-1.3185804082\H,-2.1917813743,0
.1667946062,-1.3551271204\H,-2.201347577,1.8960199674,1.1576003594\H,-
1.9278136898,0.1543985253,1.1467569447\H,2.6173573885,2.2911702578,-0.
756411117\H,-0.8896166977,-1.7834488441,-0.6719071854\H,-4.4657645445,
1.54926645,0.7353313861\H,-6.3581732068,0.4257014743,0.6581976358\H,-6
.1964160171,-1.2560376399,1.2186103746\H,-6.2095360903,-0.9071184975,-
0.5099198928\H,0.9720561258,-3.4071044165,-0.4964827066\O,4.1146929026
, -0.1396320239,-0.5800110804\H,4.3251306566,0.2719456085,0.3813857304\
H,3.3214482757,-2.6359187878,-0.4185820788\O,4.2448537784,0.564770091,
1.716711398\O,3.1528445457,-0.1440399914,2.0748074289\H,2.4056038711,0
.4767937983,2.0356881623\C,0.3122111296,3.6275860277,-0.8903517838\O,1
.3074566824,4.3438675644,-0.9108262851\C,-1.0656662741,4.2042016362,-0

.9278073111\H,-1.5514923637,3.9258232193,-1.8644057081\H,-1.6671750464
,3.8183211749,-0.1054462403\H,-0.9947360983,5.2864731383,-0.8637750043\

TS-lbj

\\O,-3.7779036557,-1.5455069735,0.3977911129\N,1.7233287645,1.718069
9933,-0.8821648624\N,-3.9449082639,0.7011362938,0.5479897456\C,-0.4346
206749,1.0505544841,-0.8284956252\C,0.4212011486,-0.0871016249,-0.6626
979336\C,-1.9260903013,0.9421039774,-0.8644590746\C,1.7506354595,0.379
633957,-0.7023848908\C,0.407883326,2.1445105623,-0.944965805\C,-2.5099
401649,0.9293348375,0.5543776084\C,0.1679295669,-1.4564459573,-0.49466
84765\C,2.8494877631,-0.4956737332,-0.557645969\C,1.2454219744,-2.3227
480791,-0.3573975168\C,2.561323792,-1.8536457227,-0.3816124976\C,-4.47
77599182,-0.5212900757,0.4296861622\C,-5.9743081437,-0.5990114247,0.34
70587059\H,-2.3744814112,1.7424854173,-1.4480381393\H,-2.188653279,0.0
004712296,-1.3487767002\H,-2.3242703801,1.8775750749,1.0535802033\H,-2
.0370994221,0.1424754478,1.1389384815\H,2.5201974232,2.3338711056,-0.9
536878221\H,-0.8471701329,-1.8301414057,-0.4688827222\H,-4.5628589657,
1.4952650075,0.5021335863\H,-6.4459837946,0.3791599863,0.4051163008\H,
-6.3327880353,-1.2277407043,1.1613085342\H,-6.2425122271,-1.0799059546
, -0.5930367794\H,1.0679986542,-3.3804158616,-0.2246616186\O,4.10476499
64,-0.0380068492,-0.6329926201\H,4.3751934855,0.362899642,0.3186140274
\H,3.3927790576,-2.5361561488,-0.2693641657\O,4.3630302124,0.684369193
9,1.643797951\O,3.2629712795,0.026310317,2.0646736378\H,2.5373918721,0
.6730149824,2.0407843381\C,0.1891281403,3.5825960051,-1.1463332386\O,1
.1551562476,4.2844852465,-1.4543888723\C,-1.1511892598,4.1386019614,-0
.9415151957\H,-1.9133850115,3.5201855921,-0.4932780607\C,-1.426808853,
5.4091838621,-1.2779668278\H,-0.6538696559,6.0244532912,-1.7260387878\
C,-2.7284702352,6.0166368707,-1.0780385109\H,-3.5016019669,5.402663657
2,-0.6300553006\C,-2.977856863,7.2817051418,-1.4257179626\H,-2.2073289
999,7.897748248,-1.8736253137\H,-3.9522134278,7.7252135594,-1.2714268356\

TS-llcF (site 4)

\\O,-3.6921092996,-1.7555433106,-0.3479398717\N,1.1490285053,2.521016
1822,0.1482049021\N,-4.2087976661,0.1261684534,0.7854148859\C,-0.85859
51279,1.5610289918,-0.2391866674\C,0.1702489136,0.6107311123,-0.506782
2188\C,-2.3154797055,1.2430864966,-0.357839895\C,1.4002570711,1.250347
7801,-0.2593066098\C,-0.213401167,2.7210591813,0.1706764744\C,-2.82830
58428,0.5618712783,0.9179425893\C,0.1394033519,-0.7386617567,-0.936041
9883\C,2.6156103,0.5843396188,-0.4371167476\C,1.3262142432,-1.40221935
29,-1.0956002726\C,2.5637622689,-0.7545012988,-0.8505736815\C,-4.54524
98438,-0.9940787076,0.1347407796\C,-6.0094438051,-1.3047133601,0.02702
92015\H,-2.9078281538,2.1301687288,-0.5619998298\H,-2.451878659,0.5557
873198,-1.1936265607\H,-2.7751616209,1.2488495626,1.7595557397\H,-2.21
13601268,-0.3054568446,1.1468042261\H,1.827997667,3.223368931,0.400245
8455\H,-4.9443944118,0.7287511742,1.1176415966\H,-6.6351189338,-0.5528

079578,0.5019140633\H,-6.1873192964,-2.2740080108,0.4915924051\H,-6.26
73734137,-1.3842081081,-1.0284759835\H,1.3602309289,-2.4345578408,-1.4
147809572\H,-0.8048233298,-1.2309778692,-1.1259471858\O,3.7357232588,-
1.3947185913,-1.0313422249\H,4.1034161982,-1.6965354353,-0.0929964052\
O,3.7820245572,1.2168643126,-0.1990869028\H,4.5124394888,0.6181406762,
-0.4163280953\O,4.2561600455,-1.8542602684,1.2979877923\O,3.138655042,
-1.2549567945,1.7475662283\H,3.4006051318,-0.3527422947,2.000979596\C,
-0.6945075186,4.0396251319,0.6039425193\O,0.1318977727,4.8931960994,0.
9081347752\C,-2.1613618455,4.3156184325,0.664592304\H,-2.576612537,4.2
925060813,-0.3442529845\H,-2.6698277467,3.5571685007,1.2590787472\H,-2
.3163861736,5.2989521566,1.0997900905\\

TS-IIcF (site 5)

\\O,3.9102201283,1.6291931692,0.1879067259\N,-1.3759032892,-2.103135
5803,-0.6366726974\N,4.1526469195,-0.5615017571,0.6769252189\C,0.71706
83364,-1.2573265908,-0.743794081\C,-0.2261749803,-0.183754111,-0.69377
7843\C,2.1970485523,-1.0447744746,-0.7671897916\C,-1.5104666222,-0.758
6955312,-0.631544873\C,-0.029086479,-2.4247385855,-0.6975466097\C,2.72
84884755,-0.8494112202,0.6586358639\C,-0.0900579471,1.2186798408,-0.69
19112452\C,-2.6730888335,0.0288315429,-0.5669603136\C,-1.2183626068,2.
0061556565,-0.6286460655\C,-2.4952323818,1.4196949889,-0.5647043322\C,
4.6453004795,0.6541320507,0.4109595416\C,6.1398531171,0.7915969382,0.4
099635217\H,2.7178717428,-1.8716422816,-1.2409075595\H,2.4120645988,-0
.1443231673,-1.3435542777\H,2.5641209611,-1.7489316371,1.2471845682\H,
2.2007308646,-0.0269440796,1.1387233139\H,-2.1202276248,-2.7840781259,
-0.6082806273\H,4.8012216007,-1.3215665294,0.8042318212\H,6.6459590434
,-0.1529050084,0.5946180987\H,6.4189177387,1.5123000512,1.1780413493\H
,6.4485899008,1.1907697509,-0.5554106636\H,-1.1513871563,3.0847914049,
-0.6228486115\H,0.8907154538,1.6738633786,-0.7369049054\O,-3.576215035
4,2.2294308532,-0.4907380669\H,-4.3774292916,1.6861366865,-0.468043756
2\O,-3.9098147615,-0.4999659783,-0.5373012152\H,-4.1994250442,-0.60861
60204,0.4591470247\O,-4.1791002651,-0.5311424332,1.8857388292\O,-3.080
4048691,0.2147660106,2.0732992004\H,-2.3452325998,-0.4092015152,2.2076
461101\C,0.3262356564,-3.8443125001,-0.6797105527\O,-0.5752508248,-4.6
765694529,-0.6159770077\C,1.7613807307,-4.2593593032,-0.7423522617\H,2
.1804431434,-3.9768130626,-1.7094892884\H,2.3415592506,-3.7658324186,0
.0366893142\H,1.8201439582,-5.3378103888,-0.6236521761\\

TS-IIcJ (site 4)

\\O,-3.6291788503,-1.854705117,-0.3340807313\N,1.066651203,2.59551585
52,-0.0263177389\N,-4.2527548594,0.045632605,0.7110591988\C,-0.9210296
243,1.5520669997,-0.2772130872\C,0.1278588392,0.6080927189,-0.47979283
04\C,-2.3683848493,1.1944739676,-0.4068380513\C,1.345181274,1.29631659
58,-0.3116754851\C,-0.2991366321,2.7612561431,0.0133149178\C,-2.893576
5468,0.53453138,0.8741152858\C,0.123834443,-0.771022084,-0.803073345\C

,2.5735881568,0.6451312468,-0.4440361456\C,1.3243963703,-1.4151315195,
-0.9330454936\C,2.5495029783,-0.7215221919,-0.7541283007\C,-4.52598626
92,-1.1011982854,0.076439119\C,-5.9737220468,-1.4488433579,-0.10989903
54\H,-2.9776477206,2.0594324653,-0.6578079228\H,-2.4693760707,0.478689
6523,-1.2240296136\H,-2.8906644203,1.2432892833,1.6992325682\H,-2.2540
579063,-0.3030836243,1.1465580158\H,1.7325656009,3.3346937775,0.142117
3006\H,-5.0196538633,0.6438080727,0.9733964862\H,-6.6412102058,-0.7075
375743,0.3223869158\H,-6.1578218219,-2.4204505336,0.3468126296\H,-6.16
76866039,-1.5358105664,-1.1787182222\H,1.3795870015,-2.4674075147,-1.1
748690416\H,-0.8104244078,-1.2989249382,-0.9388980788\O,3.7354753636,-
1.3412229805,-0.9140926561\H,4.0778580419,-1.6601941245,0.0277823791\O
,3.7275185422,1.320614261,-0.2732044655\H,4.4670124677,0.7257023874,-0
.4696149937\O,4.2022196785,-1.8259409262,1.4156149912\O,3.0847148518,-
1.2153313273,1.8479619614\H,3.3516894514,-0.3156693768,2.1043628173\C,
-0.7998000748,4.1144219395,0.2925231133\O,-0.0091598489,5.0580124601,0
.2241580945\C,-2.2021010337,4.2923251917,0.6799733919\H,-2.788928771,3
.4237686185,0.9397413998\C,-2.744682307,5.5191419488,0.7420007642\H,-2
.1452305913,6.3832198804,0.4757148114\C,-4.1158149993,5.7610684256,1.1
470546305\H,-4.7149150226,4.8998431337,1.4203040992\C,-4.6300843142,6.
992756446,1.19067786\H,-4.032968784,7.8543438379,0.9167175504\H,-5.652
4566183,7.1649655585,1.4986307072\

TS-llcJ (site 5)

\O,3.7547564105,1.7385187212,0.2401571306\N,-1.3008289093,-2.090775
7963,-0.783323471\N,4.2233584311,-0.4452869898,0.5591805911\C,0.788186
7973,-1.2302997525,-0.8220647067\C,-0.161302739,-0.1680044641,-0.70349
25799\C,2.2638194266,-0.9844737605,-0.8692796281\C,-1.4424971701,-0.75
11303338,-0.6813777838\C,0.0471343646,-2.4044452891,-0.854023306\C,2.8
301236647,-0.8593985773,0.5510319405\C,-0.032074215,1.2322363519,-0.60
78484036\C,-2.6080755837,0.0227317654,-0.5478221482\C,-1.1639753411,2.
0073881074,-0.4830269106\C,-2.4369683036,1.410705052,-0.4464982405\C,4
.5884046112,0.8320251071,0.3945292883\C,6.0597505512,1.1250473874,0.41
55543448\H,2.7910513065,-1.7588690792,-1.4207613962\H,2.4352256076,-0.
0420565555,-1.3904548361\H,2.7608144528,-1.8109364133,1.0730097854\H,2
.2502517967,-0.1263353867,1.109731425\H,-2.041976835,-2.7750417607,-0.
8027638867\H,4.9445340144,-1.1414671741,0.6588616287\H,6.6588343021,0.
2381895786,0.6059889259\H,6.2521705858,1.8698349276,1.1866918787\H,6.3
397033105,1.5555188425,-0.5455477565\H,-1.1020923293,3.0832690493,-0.4
026756896\H,0.945725997,1.6951111757,-0.6249747234\O,-3.5221997803,2.2
043149296,-0.3075568242\H,-4.31697847,1.6511943711,-0.3259008216\O,-3.
8425043023,-0.5115537301,-0.5416121154\H,-4.0664146381,-0.8033094937,0
.4352792858\O,-3.9484529801,-0.9265218835,1.8569450207\O,-2.9316123311
, -0.0817414943,2.0882764444\H,-2.1243907285,-0.6250268852,2.1156377187
\C,0.3853660119,-3.8246876017,-0.9659616544\O,-0.5256718236,-4.6312562
906,-1.1790006413\C,1.7759762747,-4.252784501,-0.7810115463\H,2.509163
639,-3.5348761776,-0.4465431579\C,2.1314375045,-5.5304198536,-0.992401
4199\H,1.3856430189,-6.2450725025,-1.3240886954\C,3.4812350718,-6.0244

501847,-0.7982971949\H,4.2317712867,-5.3137957226,-0.4708454843\C,3.79
7142561,-7.3053733491,-1.0064856294\H,4.8044163999,-7.6696298661,-0.85
53796626\H,3.0475677609,-8.0164833876,-1.3331711444\

Optimized geometries of the Cu(II) complexes

A

\O,5.3060803947,0.5419578483,-0.1116615506
\N,-1.4206045036,0.173045542,-0.0517893855\N,4.3179446621,-1.393406321
,0.5243303851\C,0.8508377297,-0.120913264,-0.3694979308\C,0.5786819685
,1.259301421,-0.227534178\C,2.1786617925,-0.7660582531,-0.570965389\C,
-0.8351630033,1.3929125114,-0.0355086857\C,-0.3978593247,-0.7353253291
, -0.2517544742\C,2.9952345316,-0.8350029642,0.7228723952\C,1.404727396
,2.4039288901,-0.2495474339\C,-1.4046334679,2.6712757029,0.1410374459\
C,0.8281993168,3.6416140186,-0.0836341515\C,-0.5701231054,3.7666505313
,0.1137342515\C,5.3738357305,-0.6769356449,0.0944474875\C,6.6553833664
, -1.4303180546,-0.1022598478\H,2.0544409996,-1.7772105477,-0.966557607
2\H,2.7491722594,-0.1963248688,-1.3110507315\H,2.4815900538,-1.4584667
07,1.4560817038\H,3.1035138101,0.1609309139,1.1546157545\H,4.431116230
5,-2.3898591326,0.6219331956\H,6.5586086488,-2.4998803357,0.0833353291
\H,7.4102173689,-1.0170563667,0.5708183121\H,7.0040088338,-1.272129304
6,-1.1249208324\H,-2.4692978086,2.7931982247,0.3033761164\H,2.47642450
25,2.3016766302,-0.3937642081\H,1.4427717992,4.5355241997,-0.097736950
8\H,-0.9931426186,4.7571616359,0.2491150385\C,-0.7746602055,-2.0988891
613,-0.3020884257\H,-0.0163058217,-2.8770281522,-0.4398737116\O,-1.974
7042047,-2.4287613562,-0.1854340213\Cu,-3.1769944557,-0.6970572994,-0.
0197254292\O,-4.4629152325,0.9538930934,0.1259826035\H,-4.2882686163,1.
.4268644225,0.9478391653\O,-4.8816874104,-1.8437105329,-0.0275117656\H
, -5.5668848804,-1.4697441984,0.5380069323\H,-4.260232056,1.5917104912,
-0.5683091805\H,-4.7007446799,-2.7207322828,0.3291947749\

C

\O,-5.300298696,0.6926027283,-0.4144388088\N,1.40750768
01,0.2496572548,0.0174741192\N,-4.2900306879,-1.3343928646,-0.35667507
84\C,-0.8530133107,0.0858949443,0.4413934329\C,-0.5044049919,1.4538222
369,0.2876299834\C,-2.2181559329,-0.4565911197,0.7035174099\C,0.900244
2547,1.508994209,0.0305260302\C,0.3452705645,-0.5942551444,0.262576637
6\C,-2.9425580548,-0.84932409,-0.5865247586\C,-1.2606579181,2.64198511
36,0.3438880211\C,1.534156857,2.75068342,-0.1735921505\C,-0.6233047586
,3.8478789194,0.1491313173\C,0.766757798,3.8954547456,-0.1103326669\C,
-5.3654948391,-0.5320865762,-0.2435056683\C,-6.6658515162,-1.201267297
9,0.0890050911\H,-2.1632690095,-1.3295628114,1.3583256992\H,-2.8126632
168,0.3011315114,1.2215384981\H,-2.389963019,-1.6373194259,-1.10103297
33\H,-2.9981693723,0.0070449246,-1.2600402282\H,-4.4070998485,-2.31096
05111,-0.1363346365\H,-6.5885571665,-2.2867003787,0.1501136211\H,-7.40

27768353,-0.9333185522,-0.670682516\H,-7.0232921034,-0.8132328253,1.04
59519303\H,2.5949884141,2.8145829873,-0.3866309652\H,-2.3288626788,2.6
021029835,0.5361434319\H,-1.1874318102,4.7738579403,0.1888980922\H,1.2
406349404,4.8595099254,-0.2665855891\C,0.6926955639,-1.9959841092,0.28
72645509\O,-0.2873710686,-2.8556779668,0.44845257\O,1.8753905903,-2.35
33915169,0.15221672\Cu,3.1310825579,-0.682632477,-0.0523910948\O,4.489
2636157,0.9024579352,-0.2437297158\H,4.3184755851,1.3704592206,-1.0694
334007\O,4.8301975774,-1.8561137595,-0.1523917164\H,5.5656834897,-1.42
38856957,0.2955756948\H,4.3384724302,1.5597667157,0.4452976397\H,4.701
8119293,-2.6918169609,0.3104086341\C,0.0379433366,-4.2593987073,0.4572
182014\H,-0.9116701308,-4.7700659879,0.592586052\H,0.4917643136,-4.541
9383737,-0.4923121255\H,0.7128600976,-4.4808495734,1.2833812647\

D

\O,5.2672279107,0.4901438177,0.5591097749\N,-1.3974384
182,0.1144018395,-0.0849252689\N,4.2789899917,-1.5474937414,0.59247180
75\C,0.8687901289,-0.1850713735,-0.390513221\C,0.5956425051,1.19704448
6,-0.2441224058\C,2.2292253419,-0.7695137989,-0.5774852861\C,-0.814889
5422,1.3349923292,-0.0621905166\C,-0.3799548792,-0.8047741378,-0.27740
75296\C,2.9232009946,-1.061347942,0.7564331351\C,1.42631151,2.33762740
76,-0.2478548368\C,-1.3831717884,2.6142570448,0.1093832529\C,0.8539837
164,3.5777395968,-0.0777534638\C,-0.5455144915,3.708278822,0.099768959
9\C,5.350816914,-0.7416642444,0.46652125\C,6.6679172465,-1.415670317,0
.2217186867\H,2.190253906,-1.6860592527,-1.1688628446\H,2.8444263445,-
0.0577857445,-1.1355620746\H,2.3650033925,-1.8126900252,1.317435695\H,
2.9565906315,-0.1567540073,1.364953131\H,4.4109518866,-2.5350582683,0.
4402505636\H,6.5995192663,-2.5033386605,0.2064224025\H,7.3696116046,-1
.1092872462,1.0002864618\H,7.0653334069,-1.0679554797,-0.7348581008\H,
-2.4499088494,2.7409290738,0.2511958925\H,2.4993599097,2.2331707148,-0
.3799972995\H,1.4739043358,4.4681945971,-0.0756207014\H,-0.9677175936,
4.6994179922,0.2335189856\C,-0.8037472875,-2.1791394137,-0.3060421004\
O,-2.0267229306,-2.4138284023,-0.1470392963\Cu,-3.1685677221,-0.710537
7286,0.036355856\O,-4.4508518943,0.9343251842,0.2275941822\H,-4.233396
8649,1.4211426763,1.0309139201\O,-4.9275386346,-1.8158065035,0.1124729
345\H,-5.5621856555,-1.3985896365,0.7054831419\H,-4.3039124794,1.56587
61596,-0.4859090461\H,-4.764620296,-2.6904596412,0.4830124064\C,0.1239
404665,-3.3203885422,-0.5206924707\H,0.5737586125,-3.2464965875,-1.514
7661023\H,0.9357632571,-3.3018596343,0.2090276626\H,-0.4196813428,-4.2
603818622,-0.4414305073\

F

\O,5.2851662027,0.4983193917,0.0723296068\N,-1.48120
63839,0.2598636903,0.309949782\N,4.2893144067,-1.4953948901,0.48325523
48\C,0.7481821321,-0.1708998674,-0.0586735535\C,0.5718206049,1.2379604
635,0.1072462165\C,2.0472698724,-0.8438490288,-0.3666861347\C,-0.81698

46743,1.4620496051,0.3039320619\C,-0.5256099388,-0.694971564,0.0728160
169\C,2.987196915,-0.9590990977,0.8355209018\C,1.4583646519,2.32743866
93,0.0838874508\C,-1.3192596457,2.7619148157,0.4524540237\C,0.95378413
83,3.6079058212,0.2423486999\C,-0.4260141823,3.8216408202,0.4224006396
\C,5.3316354897,-0.7392628952,0.0909228649\C,6.5749623695,-1.472711928
3,-0.3164468125\H,1.8837153466,-1.8370539404,-0.7914868272\H,2.5619375
188,-0.2613697125,-1.1392036623\H,2.5566622203,-1.6112015843,1.5972888
679\H,3.1380478593,0.0193491248,1.2918901882\H,4.3821190796,-2.4965514
376,0.4143349847\H,6.4804503635,-2.5565908695,-0.2508016053\H,7.399936
0379,-1.1445090163,0.3196907353\H,6.821459663,-1.1947717265,-1.3437173
397\H,-2.3810299636,2.9412642944,0.5829933327\H,2.5240720553,2.1684061
532,-0.0568852315\H,1.6276281072,4.4586157731,0.2265537482\H,-0.797466
765,4.8348194203,0.5395500749\N,-0.8835365722,-2.0701019708,0.01430830
7\C,-1.9394303501,-2.4777234068,-0.7159893243\O,-2.7379172651,-1.66429
40262,-1.2394668269\C,-0.0640724043,-3.0438878049,0.748313632\H,-0.707
6527547,-3.7577975739,1.2607529248\H,0.6137174282,-3.5822882937,0.0841
316603\H,0.5096815552,-2.5112704991,1.5003289601\Cu,-3.3230324416,0.00
58033861,-0.2287268774\O,-4.3018421685,1.2305162863,1.2342563668\H,-3.
6720911048,1.5253284401,1.9012555018\O,-5.2033590069,-0.3943061443,-0.
9892051558\H,-5.7437574321,0.4007080805,-1.0583246105\H,-4.6181092373,
2.0436425361,0.8243893914\H,-5.1254969979,-0.729280612,-1.8896363214\C
, -2.1649505284,-3.9397927631,-0.9068325555\H,-2.5251381595,-4.38040780
64,0.0276205169\H,-2.9235590269,-4.079880456,-1.6733963001\H,-1.248427
5442,-4.4593573063,-1.1887950042\\

G

\\O,-5.2860852315,0.7744642254,-0.4159525395\
N,1.3981333502,0.2601779369,0.067562432\N,-4.3454120942,-1.2850411569,
-0.3823874949\C,-0.8678598104,0.0314437565,0.4308181199\C,-0.554854081
8,1.4029568817,0.2782931177\C,-2.2462893096,-0.4868273929,0.6804248744
\C,0.8540808084,1.4988044903,0.0612626353\C,0.3610826937,-0.6311068116
,0.2817308583\C,-2.9842967261,-0.8435139704,-0.6131542854\C,-1.3516612
801,2.56821909,0.3037958622\C,1.4555776468,2.7606821064,-0.1272016528\
C,-0.7474164837,3.7900777489,0.1178146046\C,0.6504890734,3.8787588305,
-0.0962423227\C,-5.3941477516,-0.4489402242,-0.2598929018\C,-6.7166792
988,-1.0775438093,0.0667521945\H,-2.2331842665,-1.3535139257,1.3447002
93\H,-2.8200265654,0.2863319522,1.1986863222\H,-2.4609941374,-1.642686
3787,-1.1409033264\H,-3.0113412062,0.0226042986,-1.2758444049\H,-4.494
218905,-2.2612414692,-0.1804333117\H,-6.678639901,-2.1659591531,0.1133
233048\H,-7.4465032423,-0.7737898188,-0.6866331823\H,-7.0579628948,-0.
6906060172,1.0299569222\H,2.5208127813,2.8588513676,-0.2995675963\H,-2
.4237251529,2.4971249427,0.4623731037\H,-1.3401112783,4.6986293799,0.1
307201557\H,1.0979583438,4.8567643665,-0.2426536357\C,0.7642121024,-2.
0147326918,0.2989651544\O,2.0008456791,-2.25897042,0.1831224101\Cu,3.1
572697296,-0.6114734101,-0.0004004376\O,4.4712798193,1.0036454984,-0.2
311968954\H,4.2528706615,1.4803085598,-1.0401831546\O,4.9091390349,-1.
7370166392,-0.0769825555\H,5.5281457262,-1.3392961718,-0.6991389971\H,

4.3335642037,1.6455442098,0.4746289925\H,4.7278011078,-2.6184200407,-0.4220567023\C,-0.1804654986,-3.1102387291,0.4167807803\H,-1.2351434411,-2.8787971301,0.466979361\C,0.2158284646,-4.400995979,0.4522563171\H,1.2760580355,-4.633958888,0.3988781072\C,-0.6954555012,-5.5144025537,0.5568122514\H,-1.757283206,-5.2869688445,0.608580341\C,-0.2810101573,-6.788833655,0.588822689\H,0.7743659353,-7.0406496047,0.5396556975\H,-0.9860076958,-7.6090790462,0.6657823151\\

lbD

\\O,-5.2411457948,0.8189060338,-0.192784114
2\N,1.4214618113,0.3506085386,0.113413942\N,-4.2985856029,-1.216134872
8,-0.5006991934\C,-0.8434122148,0.0528760955,0.4487197905\C,-0.5719531
216,1.4379524466,0.3431551318\C,-2.20228045,-0.5312951158,0.649017263\
C,0.8347845009,1.5703025666,0.1418300568\C,0.4006157016,-0.5671085244,
0.2953319032\C,-2.9429520569,-0.733377227,-0.6762009764\C,-1.412735409
3,2.5716578513,0.4109882208\C,1.3881020597,2.8673332785,0.0194916641\C
, -0.8421804253,3.8142551025,0.2804467446\C,0.552189735,3.9595379691,0.
0871315153\C,-5.3504003267,-0.4129868771,-0.2530576327\C,-6.6761760835
, -1.0869641603,-0.0584649969\H,-2.1537791917,-1.4829011232,1.180079983
5\H,-2.7905841584,0.1497579188,1.2703223314\H,-2.412883409,-1.45543468
42,-1.2990408412\H,-2.9826277408,0.208342386,-1.225634328\H,-4.4526077
868,-2.2118291169,-0.4966459903\H,-6.6305033365,-2.1704524962,-0.16824
09191\H,-7.3860280344,-0.6813941364,-0.7826776571\H,-7.0477727194,-0.8
416789769,0.9391435445\H,-2.481604637,2.456971605,0.5605790049\H,-1.45
55765222,4.7077928651,0.3258085305\H,0.9839991382,4.9517977024,-0.0084
517201\C,0.8084018188,-1.9463241346,0.3029833869\O,2.0312561325,-2.194
8506588,0.1651171392\Cu,3.183172551,-0.5516479907,-0.0764383088\O,4.50
55441367,0.9663821958,-0.5727195512\H,4.76044301,0.8523629218,-1.49462
50865\O,4.8531730926,-1.790612789,0.0479762717\H,5.5870791248,-1.46327
58772,-0.484350826\H,3.9844613576,1.7906012405,-0.5406840944\H,4.65267
09613,-2.6648527358,-0.3048030342\C,-0.1345298141,-3.082550427,0.46716
16864\H,-0.5722270593,-3.054756181,1.4689704525\H,-0.952533199,-3.0153
945191,-0.2524013595\H,0.3958326426,-4.0243899009,0.3357095254\O,2.740
5500712,2.993713791,-0.1534832043\H,2.9772305087,3.9240763166,-0.2408553846\\

lbG

\\O,-5.2207518772,-1.56332465,0.2408198958\
N,1.4732323678,-0.8752739319,-0.1061724978\N,-4.2789917196,0.472605701
4,0.5488467663\C,-0.8044241716,-0.7202630707,-0.4464096765\C,-0.441042
3002,-2.0854007903,-0.3848682624\C,-2.2049451842,-0.2369382098,-0.6347
664727\C,0.9696160729,-2.1307688946,-0.1757328079\C,0.3972509437,-0.01
8936132,-0.2617729972\C,-2.9167057626,-0.0005481711,0.7012834772\C,-1.
2053621942,-3.2702045837,-0.4891409731\C,1.6032449182,-3.3925501886,-0.
.0719270716\C,-0.5561828122,-4.4758038136,-0.3857063804\C,0.8423626498
, -4.535303742,-0.1779442028\C,-5.330603726,-0.3316341006,0.3050647002\

C,-6.6600096483,0.3397259005,0.126136605\H,-2.2344585517,0.6752614266,
-1.2325838956\H,-2.7666260388,-0.9889033955,-1.194872041\H,-2.37633750
47,0.7420688752,1.2900824571\H,-2.9333631922,-0.9273455586,1.277086451
2\H,-4.4335659289,1.4681793159,0.5463247687\H,-6.6155785496,1.42413879
46,0.2264369656\H,-7.3566282355,-0.061783068,0.8652554202\H,-7.0483969
78,0.086857315,-0.8631010167\H,-2.278394692,-3.22304359,-0.6439152786\
H,-1.1095362624,-5.4057782693,-0.4608945877\H,1.335732911,-5.499593520
9,-0.0998197967\C,0.7318658627,1.3822369475,-0.2052638758\O,1.95414737
74,1.6820022073,-0.0765457318\Cu,3.1834597911,0.1055971943,0.124440551
2\O,4.6368298186,-1.3362510344,0.2983788455\H,5.0543403297,-1.26428969
85,1.1634824198\O,4.7612244917,1.455295087,0.325628217\H,5.4050214915,
1.1516165741,0.9751482082\H,4.1560535849,-2.1859743033,0.3021173722\H,
4.4343821083,2.2955326803,0.6663888086\C,-0.2630773274,2.4367419256,-0
.2708416598\H,-1.3048306098,2.160324153,-0.3504700953\C,0.0723415901,3
.7442057519,-0.2219580366\H,1.1193995794,4.0235533994,-0.1373124487\C,
-0.8900098011,4.8179227524,-0.2730507668\H,-1.9389928983,4.5447526211,
-0.3584420923\C,-0.5354441787,6.1095429194,-0.2203851645\H,0.506257023
,6.4049191111,-0.134521893\H,-1.2763131029,6.9003666851,-0.2599251005\
O,2.9559812437,-3.438731834,0.1324431826\H,3.2593688626,-4.3531399168,
0.1512294413\

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\O,-5.2181506653,0.8459204026,-0.177967783
2\N,1.4207030678,0.3317151909,0.1010391847\N,-4.3022359136,-1.20227366
15,-0.4797842059\C,-0.839239269,0.0334203592,0.4762617786\C,-0.5701553
161,1.4170583788,0.3561013582\C,-2.1997443724,-0.5453267141,0.67872574
86\C,0.8333344229,1.5506324867,0.123595007\C,0.4013392522,-0.588743233
8,0.3078316262\C,-2.9394738725,-0.7383498381,-0.6492228231\C,-1.408475
8596,2.549635979,0.4179353207\C,1.3785272332,2.8382344013,-0.058672337
3\C,-0.851764156,3.7930971195,0.2490693285\C,0.5338282966,3.9310640478
,0.0082660739\C,-5.3441366585,-0.3844383925,-0.2382636746\C,-6.6817333
434,-1.0378837651,-0.0539789508\H,-2.1557880826,-1.4978868917,1.207989
6088\H,-2.7852077764,0.1376974639,1.3005271527\H,-2.4165377786,-1.4675
479782,-1.2696964374\H,-2.9639910787,0.2034775752,-1.1990266969\H,-4.4
685371953,-2.1958746321,-0.4797870384\H,-6.6513611017,-2.1233599585,-0
.1484333367\H,-7.3738131963,-0.6313552711,-0.7947363765\H,-7.065287055
3,-0.7730688281,0.9339801729\H,-2.4741936413,2.4409679441,0.5905988235
\H,-1.4587259147,4.6924017252,0.2869862923\C,0.807264945,-1.963765921,
0.2971915128\O,2.0288089724,-2.2124799173,0.1289931363\Cu,3.1876710663
, -0.5622994647,-0.0478349709\O,4.5122848102,0.9980449164,-0.0708909607
\H,5.0736406209,0.9281151341,-0.8508570645\O,4.8656176218,-1.789685305
4,-0.2110151894\H,5.5345181976,-1.4146885959,-0.7947631282\H,3.9911431
74,1.815308355,-0.1900092848\H,4.6229924579,-2.6322062015,-0.611395394
6\C,-0.1332804083,-3.1014439224,0.4732694398\H,-0.5538930867,-3.077986
5922,1.4825615363\H,-0.964136047,-3.0332337047,-0.2313626889\H,0.39450
36861,-4.0430593967,0.3293134953\O,2.713720779,3.0028302565,-0.3190995
796\H,2.9140993241,3.943225104,-0.4020221872\O,1.1190014715,5.15450588

49,-0.1842252078\H,0.4554263797,5.8497012217,-0.1270676295\\

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\\O,-5.0610487628,-1.6691341501,0.490608835
2\N,1.4703467111,-0.8483353913,-0.1859673926\N,-4.2855425346,0.4557997
616,0.5866408153\C,-0.812545362,-0.6646578936,-0.4849764066\C,-0.46094
94576,-2.0333524505,-0.4470608662\C,-2.2150430118,-0.1754161251,-0.638
7831871\C,0.9550195105,-2.095987048,-0.2694601406\C,0.3982048943,0.024
3641474,-0.3090303732\C,-2.8857267879,0.0991850329,0.7108429593\C,-1.2
313187829,-3.2116695251,-0.5529331277\C,1.5883584072,-3.3539570369,-0.
2270141019\C,-0.5943042757,-4.4257081565,-0.488350975\C,0.8088073236,-
4.4917589696,-0.3284369617\C,-5.2735073799,-0.4501318987,0.4537146888\
C,-6.6601901196,0.0908244749,0.2683647936\H,-2.2611770259,0.7223049815
, -1.258616663\H,-2.7976170869,-0.9388510599,-1.1601796131\H,-2.3795778
863,0.9167352409,1.226440739\H,-2.812778684,-0.7847727101,1.3463579829
\H,-4.5203900586,1.431296313,0.4940228936\H,-6.7056863971,1.1796631344
,0.2807274263\H,-7.2996419035,-0.305112803,1.0604591453\H,-7.051321892
2,-0.2749539199,-0.6837381747\H,-2.3076171492,-3.1626296517,-0.6788437
966\H,-1.1480351127,-5.356550417,-0.5602933812\C,0.7473344848,1.415206
7591,-0.2156769747\O,1.9660441158,1.6976949984,-0.0038085513\Cu,3.1575
928543,0.1184539461,0.2437739111\O,4.494859489,-1.3759837681,0.6465011
545\H,4.7273679387,-1.3577599201,1.5809782183\O,4.800454313,1.40078337
88,0.4553245962\H,5.4366399261,1.0745870073,1.1010023595\H,4.030355410
8,-2.222255984,0.497699994\H,4.5173060647,2.2588108535,0.7903646468\C
, -0.2226168441,2.4860736028,-0.3524717766\H,-1.2559788809,2.2259774458
, -0.5340696863\C,0.125760884,3.7880076131,-0.265545739\H,1.1644259903,
4.0499270227,-0.0812495069\C,-0.8097638055,4.8774966041,-0.4052507542\
H,-1.8507522021,4.6209746239,-0.5867218429\C,-0.4426592918,6.163909885
3,-0.3198279647\H,0.59109199,6.4449145422,-0.1407264574\H,-1.165716347
8,6.9646733736,-0.4278038466\O,2.9491371155,-3.4500676113,-0.098611628
8\H,3.2033693918,-4.380340393,-0.0554693532\O,1.4802031235,-5.68296985
07,-0.2685913204\H,0.8598701346,-6.4182786645,-0.3084746156\\

Optimized geometries of the Cu(I) complexes

A

\\O,5.4714148107,0.6144527764,0.2090836457\N,-1.2017521039,-0
.1152096951,-0.2503207703\N,4.5525646221,-1.4314033538,0.5187808194\C,
1.0894055262,-0.2590530457,-0.5379739917\C,0.7382055892,1.1032738037,-
0.4031885732\C,2.4730908793,-0.7979511702,-0.6961794588\C,-0.679496894
1,1.1357829028,-0.233083693\C,-0.1241807808,-0.9578286806,-0.432215415
9\C,3.1823431217,-0.9731329183,0.6496898683\C,1.4788069151,2.305608046
6,-0.410791006\C,-1.3469077079,2.3695319677,-0.0774661584\C,0.80924770
73,3.4996888242,-0.2568881458\C,-0.5991126033,3.5266451384,-0.09087380
24\C,5.5960896859,-0.6157928659,0.2806308881\C,6.9350147295,-1.2713087

153,0.1125135955\H,2.4639732027,-1.7583947642,-1.217029433\H,3.0608268
146,-0.1090201723,-1.3104857471\H,2.6481357288,-1.7042834765,1.2586124
86\H,3.1857480324,-0.0293068333,1.1969772537\H,4.7196929267,-2.4248466
131,0.5190606969\H,6.9049838258,-2.3548801113,0.2275339675\H,7.6260828
236,-0.8500996569,0.8458275101\H,7.3189848297,-1.0253968968,-0.8802204
361\H,-2.4250094235,2.3980347872,0.0506743161\H,2.5581989921,2.2865082
189,-0.5346477963\H,1.3592956552,4.4351275395,-0.2596357597\H,-1.09519
02425,4.4848988367,0.0284083817\C,-0.2503226073,-2.3889774989,-0.49458
62468\H,0.6988590376,-2.9273179019,-0.6615222262\O,-1.2927332363,-3.03
66260865,-0.3791164692\Cu,-3.0402493917,-0.5880421844,-0.0171874876\O,
-6.4797137474,1.1394797467,0.9259371867\H,-6.1339308064,1.5567763008,1
.7206816759\O,-4.9625459875,-1.0530148882,0.2266480307\H,-5.4951165826
, -0.2754185812,0.4973841199\H,-6.4247198388,1.8261032456,0.254101044\H
, -5.0804345022,-1.7025390252,0.9260771314\

C

\O,-5.4887251313,0.9026972107,-0.5190761286\N,1.263758169,0.2
260306859,-0.0084811578\N,-4.5069574437,-1.1367122677,-0.3952303365\C,
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317727,-0.5115890632\H,0.0531404482,-4.4823527395,1.2461927997\

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,-0.9671646,-0.2379993378,0.4774568213\C,-0.5857608782,1.1157059345,0.3044613834\C,-2.3883237723,-0.6624080396,0.6725789919\C,0.8254296896,1.1184663875,0.1154784062\C,0.2311169822,-0.9696401485,0.3771082535\C,-3.1274741778,-0.8392700385,-0.6570911674\C,-1.3025467722,2.3317186342,0.2897855353\C,1.5155378203,2.3325703479,-0.0854959374\C,-0.6127451946,3.5096931449,0.0943130466\C,0.7923408701,3.5064022237,-0.0926526763\C,-5.5089532555,-0.3177082411,-0.2672830405\C,-6.882725543,-0.8827425284,-0.0569954132\H,-2.4658459731,-1.5833232077,1.2499765265\H,-2.9096485399,0.1093294755,1.2473135863\H,-2.6525395664,-1.6184374556,-1.2553773504\H,-3.0820476233,0.0859927864,-1.2337106864\H,-4.7487369957,-2.1856052219,-0.4471352648\H,-6.9180523021,-1.9704534233,-0.1172085098\H,-7.553815604,-0.4596285779,-0.8076297299\H,-7.2442787595,-0.5653401729,0.9237148048\H,2.5931457578,2.3351630897,-0.2300617139\H,-2.3806270425,2.3389495141,0.427662815\H,-1.1461602775,4.4548803333,0.080377027\H,1.3056941999,4.4508256106,-0.2450076023\C,0.4669795984,-2.4134689614,0.4747291962\O,1.6120344769,-2.871687607,0.3949369512\Cu,3.1616189082,-0.607865275,-0.0683412251\O,5.7784011023,1.8681142705,-0.7458410481\H,4.9091401832,2.2812687135,-0.7280347472\O,5.1313520876,-0.7810185595,-0.3279502649\H,5.4572284874,0.1291176097,-0.4922751667\H,6.2468292473,2.2713699094,-0.0086655877\H,5.3442170063,-1.2777679999,-1.1241006115\C,-0.6773221284,-3.363089928,0.6810150061\H,-1.136381232,-3.1992775243,1.6598829863\H,-1.452968365,-3.2324813787,-0.0753328661\H,-0.3026187254,-4.3851331857,0.6379724974\

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30713,-7.6716381785,0.5365279969\

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72445\H,0.595890761,-4.8689957089,-0.3793150841\C,-0.3121353861,2.1414
713827,-0.4130084243\O,0.5623969322,2.9569801645,-0.7469116099\Cu,2.84
02529861,1.4485318495,-0.1121898048\O,5.469291765,0.0309375157,1.47314
17981\H,4.8201893856,-0.4957780002,0.9812792669\O,4.6019068345,2.34467
38861,0.2657590982\H,5.0696711795,1.6457651159,0.7686001887\H,6.321170
9643,-0.3359271377,1.220864012\H,4.5046387709,3.0845605766,0.872640312
5\C,-1.6535967614,2.6125142887,-0.0253141536\H,-2.3224818132,1.9243334
964,0.474300609\C,-2.0566636607,3.8799681911,-0.2362006909\H,-1.384134
5381,4.57431838,-0.7347624293\C,-3.3512277351,4.3905800852,0.157854260
6\H,-4.0266780759,3.698059946,0.655066337\C,-3.7371066723,5.6546449697
, -0.0611834317\H,-3.0833909479,6.3672747582,-0.5560312225\H,-4.7144855
671,6.0085897044,0.2485443084\O,3.6621940105,-1.5159625472,-0.23386232
53\H,4.2454149702,-2.2799559382,-0.3272118811\O,3.1640767099,-4.157059
146,-0.2558998889\H,2.8733067546,-5.0705727496,-0.340025319\